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During the period covered by this grant, we conducted research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We studied both local refinement methods and methods of lines techniques using properly nested and overlapping grids. The geometric modeling capabilities of our procedures were improved thaough the use of finite quadtree and octree encoding schemes; parallel versions of adaptive procedures on shared-memory computers were developed; and variable-order finite element methods to be used with adaptive p- and hp-refinement were created.

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Principal Investigator: Joseph E. Flaherty

Department of Computer Science

Rensselaer Polytechnic Institute

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ABSTRACT

During the period covered by this grant, we conducted research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We studied both local refinement methods and methods of lines techniques using properly nested and overlapping grids. The geometric modeling capabilities of our procedures were improved through the use of finite quadtree and octree encoding schemes; parallel versions of adaptive procedures on shared-memory computers were developed; and variable-order finite element methods to be used with adaptive p- and hp-refinement were created.

1. Progress and Status of the Research on Adaptive Numerical Methods.

During the period covered by this grant, we conducted research on the development and analysis of finite difference and finite element methods for steady and transient partial differential systems in one, two, and three space dimensions. A list of publications is given in Section 3 and some of our key findings are highlighted below.

Using a local refinement finite difference or finite element method, error estimates of solutions generated on a coarse spatial grid for one time step are used to create finer space-time subgrids in regions where greater resolution is needed. The problem is recursively solved on these finer grids until prescribed accuracy criteria have been satisfied. The process continues in this manner proceeding from coarse time step to coarse time step. Flaherty et al. [2-4] reported on a two-dimensional local refinement procedure that uses uniform space-time grids with finer grids overlapping coarser ones. Solutions on overlapping grids at the same level of our tree data structure are obtained using the Schwarz alternation principle, which appears to be efficient and robust. We introduced the concept of a "megagrid" that contains all overlapping grids of the same and/or finer levels of the tree. The megagrids greatly simplify data management and searching problems associated with overlapping grid methods. The procedure used to solve linear systems on the various grids has been improved by using an incomplete orthogonalization procedure.[1] This and additional improvements to the clustering algorithm that is used to define local grids have been reported in a paper [3] that appeared as part of the proceedings of the workshop on *Adaptive Computational Methods for Partial Differential Equations* that was organized by J. E. Flaherty, M. S. Shephard, and J. D. Vasilakis and held at the Rensselaer Polytechnic Institute. A more detailed analysis of the method will appear shortly [4].

The success of high-order methods and adaptive hp-refinement techniques on elliptic

[1] Y. Saad, "Practical Use of some Krylov Subspace Methods for Solving Indefinite and Nonsymmetric Linear Systems," *SIAM J. Sci. Stat. Comput.*, 5 (1984), pp. 203-228.

systems has led us to investigate analogous procedures for time-dependent problems. The transient situation is far more difficult than the steady one due to the need to balance spatial and temporal errors combined with the difficulty of obtaining reasonable estimates of the global temporal discretization error. Martin Berzins of Leeds University visited Rensselaer during the course of this grant. He is an expert on global temporal error estimation and high-order (spectral) approximation. In collaboration, we have been investigating the use of singly implicit Runge-Kutta (SIRK) methods and backward difference formulas (BDFs) with high-order restarting to achieve high temporal orders of accuracy. A report on a method for one-dimensional problems that combines h- and p-refinement will be submitted for publication shortly.

Local mesh refinement finite volume software for hyperbolic systems [1, 5, 6] has been combined with finite quadtree mesh generation procedures for the solution of two-dimensional problems, respectively. These studies combine motion of a coarse "base" mesh with local temporal and spatial mesh refinement. In contrast to the overlapping grid procedures, fine grids are properly nested within coarse mesh cells; thus, reducing interpolation difficulties at mesh interfaces. The quadtree mesh generation procedures are used to create the initial grids, respectively, on complicated domains. The mesh generation techniques are completely automatic and their tree data structure nicely matches the tree structure that we employ for local refinement. Two-dimensional codes have been written and are being used to solve transonic flow problems about airfoils, wings, and wing-body combinations. A three-dimensional version is under development. Parallel versions of the adaptive procedure have been implemented on shared-memory MIMD computers [7]. Several static and dynamic load-balancing strategies indicate the effectiveness of using adaptive methods in parallel computational environments. One static strategy utilizes a posteriori error estimates that are furnished as part of our adaptive mesh-refinement process to calculate approximations of the computational effort needed to reduce the error estimate to prescribed levels. These work estimates are then used to schedule processors to balance loading.

A parallel adaptive procedure for solving elliptic problems on shared-memory computers has also been developed [7, 8]. Our technique combines quadtree mesh generation with h- and p-refinement. A preconditioned conjugate gradient method with either an element-by-element (EBE) or a symmetric successive over-relaxation (SSOR) preconditioner is used to solve the linear systems that arise from the finite element discretization. "Coloring" of arbitrary finite element meshes in order to avoid critical sections is a complex operation. By exploiting the underlying quadtree grid structure, we have developed procedures to color quadrants of the tree with six or eight colors. Four is provably the minimum number of colors that are needed; however, the six- and eight-color schemes have linear time-complexity. The six-color scheme performs significantly better than the eight-color scheme. Edge coloring schemes are being developed for higher-order finite element approximations.

We are anxious to have our adaptive software used by scientists and engineers and, in order to make it easier for them to do so, we developed a symbolic interface to our software [2, 3]. Users of this interface can describe their problems in a relatively natural language. Appropriate solution techniques are suggested after some dialogue with the user about the peculiarities of the problem at hand and code for evaluating functions, Jacobians, boundary conditions, etc., is generated automatically from the symbolic input and is linked with the relevant adaptive procedures.

2. Interactions

Professor Flaherty lectured and/or visited the following conferences and organizations during the period covered by this report:

J. E. Flaherty held technical discussions with Dr. John Walter of the U. S. Army's Ballistics Research Laboratory at the Rensselaer Polytechnic Institute, March 13, 1989.

J. E. Flaherty attended the *Seventh International Conference on Finite Element Methods in Flow Problems,* University of Alabama in Huntsville, April 3-7, 1989. He presented lectures on "Experiments with Mesh Moving and Local Refinement Algorithms for Hyperbolic Systems" and "Solving Compressible Flow Problems Using Finite Quadtree and Octree Grids."

J. E. Flaherty held technical discussions with Dr. Alex Woo of the NASA Ames Research Center at the Rensselaer Polytechnic Institute, April 25, 1989.

J. E. Flaherty and B. K. Szymanski (of Rensselaer's Computer Science Department) hosted the *Fifth Parallel Computing Circus,* April 28, 29, 1989 at the Rensselaer Polytechnic Institute. Approximately seventy scientists attended this symposium and featured twenty-one talks by faculty and graduate students.

J. E. Flaherty attended the *Fourth International Conference on Supercomputing* at Santa Clara, May 1-5, 1989. He presented an invited lecture on "An Environment for the Parallel Solution of Parabolic Partial Differential Equations."

J. E. Flaherty and R. Biswas, a graduate student supported by this grant, attended the *Seventh Army Conference on Applied Mathematics and Computing* at West Point, June 6-9, 1989. He lectured on "Numerical Experiments in Adaptive Mesh Methods."

J. E. Flaherty lectured on "Adaptive H-, P-, and R-Refinement Finite Element Schemes for Parabolic Partial Differential Systems" at the *SIAM National Meeting* in San Diego, July 17-21, 1989.

J. E. Flaherty held technical discussions with Dr. John Walter of the U. S. Army's Ballistics Research Laboratory at the Rensselaer Polytechnic Institute, September 25, 1989.

J. E. Flaherty and P. K. Moore, a Postdoctoral Fellow supported by this grant, attended the workshop on *Reliability in Computational Mechanics* in Austin, October 26-28, 1989. J. E. Flaherty presented an invited lecture on "Parallel Computations with Adaptive Methods for Partial Differential Equations."

J. E. Flaherty visited with Dr. Martin Berzins and lectured at the University of Leeds on "Adaptive H-, P-, and R-Refinement Finite Element Schemes for Parabolic Partial Differential Systems," November 28-29, 1989.

J. E. Flaherty and M. Benantar, a graduate student supported by this grant, attended the *Fourth SIAM Conference on Parallel Processing for Scientific Computing* in Chicago, December 11-13, 1989. He lectured on "Parallel Element-by-Element Techniques for Elliptic Systems using Finite Quadtree Meshes."

J. E. Flaherty lectured on "Adaptive Methods Employing Quadtree Structures for Partial Differential Equations" at Tulane University, February 2, 1990.

J. E. Flaherty attended a DARPA Meeting on "The Direct Simulation of Turbulence" in San Diego on May 14, 1990.

3. List of Publications.

1. D.C. Arney and J.E. Flaherty, "An Adaptive Local Mesh Refinement Method for Time-Dependent Partial Differential Equations," *Applied Numerical Mathematics* 5 (1989), pp. 257-274.

2. P.K. Moore, C. Ozturan, and J.E. Flaherty, "Towards the Automatic Numerical Solution of Partial Differential Equations," *J. Maths. and Comput. in Simulation* **31** (1989), pp. 325-332.

3. J.E. Flaherty, P.K. Moore, and C. Ozturan, "Adaptive Overlapping Grid Methods for Parabolic Systems," in J.E. Flaherty, P. Paslow, M.S. Shephard, and J.D. Vasilakis, Eds., *Adaptive Computational Methods for Partial Differential Equations, II* SIAM, Philadelphia, 1989, pp. 176-193.

4. P.K. Moore and J.E. Flaherty, "Adaptive Local Overlapping Grid Methods for Parabolic Systems in Two Space Dimensions," Technical Report 90-5, Department of Computer Science, Rensselaer Polytechnic Institute, January 1990. Also, submitted for publication.

5. D.C. Arney, R. Biswas, and J.E. Flaherty, "An Adaptive Mesh Moving and Refinement Procedure for One-Dimensional Conservation Laws," Technical Report 90-6, Department of Computer Science, Rensselaer Polytechnic Institute, January 1990. Also, submitted for publication.

6. D.C. Arney and J.E. Flaherty, "An Adaptive Mesh-Moving and Local Refinement Method for Time Dependent Partial Differential Equations," in *ACM Transactions on Mathematical Software,* Vol. 16, No. 1, March 1990, pp. 48-71.

7. M. Benantar, R. Biswas, J.E. Flaherty, and M.S. Shephard, "Parallel Computation with Adaptive Methods for Elliptic and Hyperbolic Systems, in *Computer Methods in Applied Mechanics and Engineering,* **82** (1990) pp. 73-93.

8. M. Benantar and J.E. Flaherty, "A Six-Color Procedure for the Parallel Solution of Elliptic Systems Using the Finite Quadtree Structures," in J. Dongarra, P. Messina, D. C. Sorensen and R. G. Voigt, Eds., *Proceedings of the Fourth SIAM Conference on Parallel Processing for Scientific Computing*, SIAM, Philadelphia, 1990, **23**, pp. 231-236.